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# Computer Perception of Constitutional (Topological) Symmetry: TOPSYM, a Fast Algorithm for Partitioning Atoms and Pairwise Relations among Atoms into Equivalence Classes

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An algorithm for the perception of constitutional symmetry in molecules (graphs) is presented, which partitions not only atoms (vertices) but also all pairwise relations among skeleton atoms into equivalence classes. The method works without canonical numbering, essentially by raising the connectivity matrix of the arbitrarily numbered molecule (graph) to its second, third, etc. power and evaluating the entries in these higher order matrices.

When developing a computer program for the machine generation of systematic (IUPAC) names for polycyclic organic compounds,[1] we encountered the more fundamental problem of computer perception of symmetry. For example, how many different pairs of potential bridgeheads are present in the bis- and trissecododecahedranes **1–4** (Figure 1): in particular, which pair is equivalent to which other pair? This question is obviously much harder to answer than the question of how many different kinds of atoms are present in these same compounds. Whereas several computer methods exist for the purpose of partitioning atoms in a molecule into equivalence classes[2-8] and some work has also been done on the detection of the identity of bonds,[4,9] no general method appears to be available to treat pairwise (or even higher) relations among the atoms.[10]

The symmetry properties of a molecule (as well as all other properties) are obviously encoded in its structure; the difficulty lies in the decoding process. Since the structure (more precisely, the constitution) can be represented by a connectivity (adjacency) matrix[11] and since the constitutional symmetry is a very fundamental and simple property, we expected that it could be derived by some simple mathematical manipulation of the connectivity matrix. This turned out to be the case, and we report herein on an algorithm (and the computer program TOPSYM based on it) that finds equivalence classes of atoms and pairs of atoms by a purely mathematical approach. That is, we do not need a canonical numbering,[3,5,6] nor do we need to assign numbers to atomic properties (as was done in a somewhat arbitrary manner in some recent solutions of the atom equivalence problem[8]).

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